

Approximate Calculation of Geometric-Cluster Combinatorics in 2D and 3D Ising Models

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We found [1] that distribution of geometric clusters in 2D and 3D Ising models may very well be approximated by an expression, analytic in 2D:

$$n(v, s) = g(v, s) \exp\left(-\frac{cs}{T} + v_{ex} \frac{\Delta F_l}{T}\right) (1 - \sum v) \quad (1)$$

Here v and s mean volume and surface area (area and perimeter in 2D) of a cluster, g is the cluster combinatorial factor, $c = 2$ is the surface energy coefficient; v_{ex} , numerically equal to the sum of volume and surface of a cluster, accounts for the number of cites that a given cluster excludes from the lattice; F_l is the Ising free energy per spin of the lattice; $\sum v$ means the average volume per spin occupied by all the clusters which is related to spontaneous magnetization, and T is temperature.

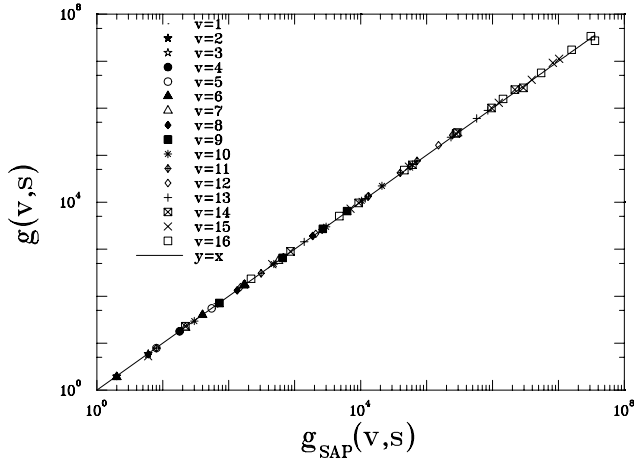


FIG. 1: Correspondence of extracted 2D Ising combinatorials to the exact self-avoiding-polygon (SAP) combinatorics.[2]

Eq.(1) may be used to extract the combinatorials $g(v, s)$ by fitting the geometric-cluster distributions obtained from a 2D Ising simulation. This has been done, and the results are shown in Fig.1. In Fig.1 we compare the $g(v, s)$ values obtained from our fit to the exact values calculated by Jensen

[2]. The agreement is better than 5%, while the values of g vary over 8 orders of magnitude.

This technique can be applied to Ising calculation in 3D where to the best of our knowledge no published size-and-area enumeration of 3D SAP exists. Enumeration by size only was reported up to $v = 17$ [3].

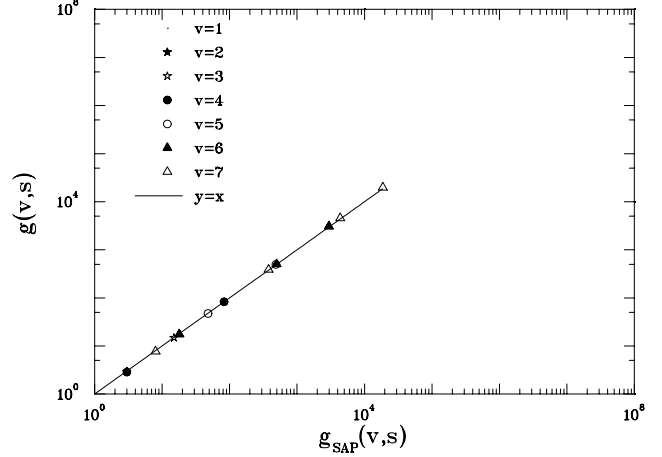


FIG. 2: Correspondence of extracted 3D Ising combinatorials to the exact self-avoiding-polyhedra (SAP) combinatorics. The exact data were obtained by one of us (JH) using direct enumeration.

Our method allows one to estimate the Ising combinatorics for practically any cluster in terms of surface and cluster size with 1 – 5% accuracy within a reasonable CPU time (hours).

REFERENCES

- [1] Previous report.
- [2] Iwan Jensen. Private communications.
- [3] Achim Flammenkamp. On-line Encyclopedia of Integer Sequences.